Instanton approach to the decay of a metastable quantum state

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Abstract: The escape transition due to quantum tunnelling of a particle from a metastable region, created by a cubic potential, is studied. Finding this amplitude is reduced to the computation of a Feynman path integral. This calculus has been carried out using the instanton method, which demands to rotate the time coordinate along the imaginary plane. The results obtained show that the ground state energy has actually an imaginary part (fact that is actually related to the metastability of the system) and allows to find the decaying rate of the metastable state.

I. Introduction

Quantum tunnelling is a quantum phenomenon through which a particle can surpass a potential barrier even if its total energy is lower than that of the barrier. It is known to be of prime importance in many different quantum-sized physical phenomena. For instance: heavy nuclei that decay by an alpha decay process, nuclear fusion processes [1], scanning tunnelling microscopy and quantum devices in solid-state physics [2], Bose-Einstein condensates [3], a wide range of chemical reactions [4], in biology [5], etc.

It can be taken even further if we study it via quantum field theory (QFT) formalism: now a scalar field positioned in a local minimum of its potential can tunnel to an absolute minimum. This is, the study of false vacuum states [6],[7].

There is a wide range of methods to study this phenomenon (each one convenient for different specific cases) such as the WKB approximation, scattering methods, the instanton method, etc. ([8], [9]). Path integral methods are useful because of their quite "easy" generalization to problems with arbitrary dimensions. Moreover, they are one of the few methods that are nonperturbative. Apart from that, they allow to control very well the level of approximation that is being made and, thus, it is easier to carry a classical limit. The method we are going to use in this work, the instanton method, starts from a Feynman path integral and, thus, it will have all these advantages.

II. Feynman Path integral

Suppose that a particle is confined by a potential. We want to evaluate the transition amplitude of it tunnelling through the barrier that is confining it. It can be easily seen that this object actually matches with the matrix elements of the time evolution operator, namely

$$\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | U(t_f, t_i) | x_i \rangle. \quad (1)$$

This element turns out to be computable as the Feynman's path integral ([10]) over all the possible trajectories (classical and quantum) which the system could go through in order to evolve from the initial state to the final state (since, in quantum mechanics, one must take into account all the paths that are possible, not just one, as classically).

This is:

$$\left\langle x_f \left| e^{-\frac{i}{\hbar}TH} \right| x_i \right\rangle = N \int \mathcal{D}x \, e^{\frac{i}{\hbar}S[x]}, \quad (2)$$

where $\mathcal{D}_x$ stands for the integration over all the possible paths (all of them starting from the same initial state and ending up at the same final state). $S[x]$ is the action of each trajectory and $T \equiv t_f - t_i$.

III. Imaginary time

The action of each trajectory is given by

$$S[x] = \int_{-\frac{T}{2}}^{+\frac{T}{2}} dt \left(\frac{1}{2} m\dot{x}^2 - V(x) \right). \quad (3)$$

Note that if a classical trajectory is allowed, then Eq. (3) will have an extreme for that trajectory. Thus, we will be able to expand our total action around it, since the main contributions to the integral come from the paths close to the classical one, while the distant ones cancel each other. However, in quantum tunnelling there is no classical trajectory, so, to continue, one must take some additional steps, which will finally allow us to use such expansion, as it will be seen below.

In order to compute the transition amplitude in Eq. (2) using this method, a rotation to imaginary time can be done: $t \to t' = -i\tau$. This is called "Wick rotation". Note that we moved from the Minkowski space to an Euclidian space:

$$x^\mu = (t, \vec{x}) \to (-i\tau, \vec{x}),$$
$$x_\mu x^\mu = (t^2 - \vec{x}^2) \to -(\tau^2 + \vec{x}^2). \quad (4)$$

Because of this change in the temporal coordinate, Eq. (2) becomes

$$\left\langle x_f \left| e^{-\frac{1}{\hbar}TH} \right| x_i \right\rangle = N \int \mathcal{D}x \, e^{-\frac{1}{\hbar}S_E[x]}, \quad (5)$$

where

$$S_E[x] = \int_{-\frac{T}{2}}^{+\frac{T}{2}} d\tau \left(\frac{1}{2} m\dot{x}^2 + V(x) \right) \quad (6)$$

is the Euclidean action.

It will be interesting later to expand the left-hand-side of Eq. (5) in a complete set of energy eigenstates:

$$\left\langle x_f \left| e^{-\frac{1}{\hbar}TH} \right| x_i \right\rangle = \sum_n e^{-\frac{E_n T}{\hbar}} \langle x_f | n \rangle \langle n | x_i \rangle. \quad (7)$$

We can see here that the imaginary argument of the exponential turned into a real one by implementing this change. Moreover, now the trajectory is governed by a potential $-V(x)$, and not $+V(x)$. This is the key point of this method: by implementing a Wick rotation, we managed to change the sign of our potential. This has a direct consequence to the trajectory, as it follows.
If the potential had a barrier that the particle could classically not cross, now, in the inverted potential, that barrier will have turned into a well. Thus, now the particle is able to move classically along the previously forbidden region.
More specifically, the potential barrier that is studied in this work comes from a cubic potential ($V(x) \equiv V_c(x)$), which has the following expression:

$$V_c(x) = \frac{1}{2}mw^2x^2\left(1-\frac{x}{x_0}\right). \qquad (8)$$

It can be seen in *Fig. 1* that, as said before, the particle starting at the initial point $x_i = 0$ has a classically allowed trajectory along the *x* axis, while before the Wick rotation clearly hadn't, since it is assumed that the total energy of it is inferior than the relative maximum at $x_e = \frac{2}{3}x_0$ (i.e. $E < V_c\left(\frac{2}{3}x_0\right)$).

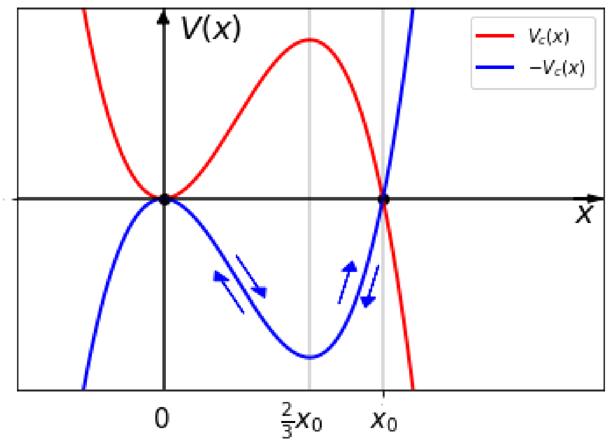

FIG.1: Qualitative illustration of the cubic potential, Eq. (8), before (red) and after (blue) the rotation to imaginary time. For the inverted potential, it is shown the classical trajectory that would follow a particle starting at x=0. Note that at x_0 it bounces back.

The action $S_E[x]$ must present, therefore, a minimum for the classical trajectory discussed. Following ([7], [8]), an expansion around this trajectory and therefore, of the action, can be done. Together with this, the oscillations around the classical trajectory, $\eta(t)$, can be expressed as a linear combination of the eigenfunctions of the following operator $-\frac{d^2}{d\tau^2}+V''(x_{cl})$,

$$x(\tau) = x_{cl}(\tau) + \sum_n c_n\psi_n. \qquad (9)$$

So, it is finally obtained that Eq. (5) can be written as ([8]):

$$\left\langle x_f \left| e^{-\frac{1}{\hbar}TH} \right| x_i \right\rangle = \frac{Ne^{-\frac{1}{\hbar}S_0}}{\sqrt{\det\left(-m\frac{d^2}{d\tau^2}+V_c''(x_{cl})\right)}}, \qquad (10)$$

where $S_0 \equiv S_E(x_{cl})$ is the action for the classical trajectory, governed by the potential $-V_c(x)$, and N is just a normalization factor. The determinant comes in fact from the following expression:

$$(\det(B))^{-1/2} = \int \prod_{n=0} \frac{dc_n}{\sqrt{2\pi\hbar}}\, e^{-\frac{1}{2\hbar}\sum_{n=0}\lambda_n c_n^2}, \qquad (11)$$

where B is the operator that appears at the denominator of Eq. (10), dc_i stand for the integration over all possible paths and λ_n are the eigenvalues of the operator B.
So now, the "only" things that remain to be done is the computations of the exponent factor ($e^{-\frac{1}{\hbar}S_0}$) and the determinant value. It will be shown how to do it on the next sections. Note that here the determinant could take a negative value and thus the transition amplitude would be imaginary. Even, it could take a value of zero and the amplitude would diverge. This is, in fact, our case of study and it will be further studied in the next sections.

IV. Classical trajectory and instantons. The exponential factor.

Let us focus for now on the exponential factor, which comes from the contribution of the classical trajectory, that follows the inverted potential ($-V_c(x)$). The action of this system is:

$$S_0 \equiv S_E(x_{cl}) = \int_{-\infty}^{+\infty} dt\left(\frac{1}{2}m(\dot{x_{cl}})^2 + V(x_{cl})\right) \qquad (12)$$
$$= 2\int_{-\infty}^{0} dt\, 2V(x_{cl}) = 2\int_0^{x_0}\sqrt{2mV(x_{cl})}\,dx_{cl}.$$

Note here that the action can actually be computable directly by knowing the potential and there is no need to know the actual classical trajectory. By plugging the potential of Eq. (8) into Eq. (12), it is obtained:

$$S_0 = \frac{8mw(x_0)^2}{15}. \qquad (13)$$

One can also obtain an expression for the classical trajectory, by using $\frac{\delta S_E}{\delta x_{cl}} = 0$, which gives:

$$m\ddot{x} - V'(x) = 0. \qquad (14)$$

Solving this equation we find the classical trajectory:

$$x_{cl}(\tau) = x_0 \,\mathrm{sech}^2\left[\frac{w}{2}(\tau - \tau_c)\right], \tag{15}$$

where τ_c is an integration constant that will be discussed below. In *Fig. 2* we can see that the trajectory is a bounce between the starting point ($x = 0$) and a returning point x_0. This can also be seen in *Fig. 3* where the Lagrangian of this trajectory is shown. Two peaks can be observed for the Lagrangian. That should not bother us, as we know that a bounce occurs at τ_c and, thus, the velocity at that point is zero. Moreover, the duration of the bounce can be obtained analysing the "width" in time of this trajectory, which turns out to be $\Delta t \sim \frac{1}{w}$ (small quantity). So we see that this solutions are quite localized in time, around τ_c. This is why they are commonly called "instantons", because of their similarities with "solitons", but now centered in time. It is now when we can recover the integration constant τ_c: we see that the value of this constant is actually irrelevant to the physics of the system, because it only changes in time (imaginary time) the center of the phenomena. This is actually quite important, so it directly traduces into the time invariance of the system.

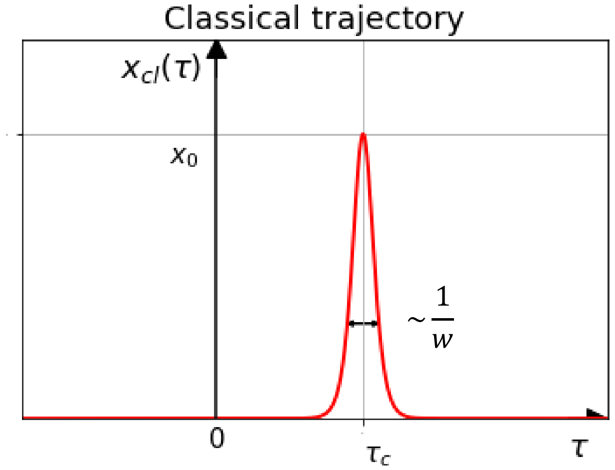

FIG.2: Classical trajectory for the instanton solution. As we can see, it is localized around τ_c, parameter that could take any value.

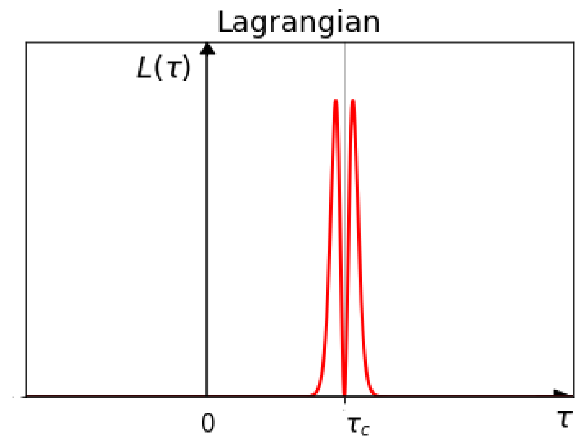

FIG.3: Classical Lagrangian for the instanton solution. It's also localized around τ_c.

We can see how, indeed, the system stays still most of the time and, near τ_c, performs the bounce for a short period of time.

V. Calculation of the determinant: zero eigenvalues and complex energies

It can be easily seen that, as the classical trajectory must obey Eq. (14), the classical velocity, namely $\frac{dx_{cl}}{dt}$, is actually an eigenfunction with zero eigenvalue of the operator B (of which we intend to calculate its determinant). So, we can define the normalized wavefunction with that eigenvalue as follows:

$$\left[m\frac{d^2}{d\tau^2} - V''(x_{cl})\right]\frac{\mathrm{dx_{cl}}}{\mathrm{dt}} = 0 \rightarrow$$
$$\rightarrow \psi_0 \equiv \left(\frac{\mathrm{S_0}}{\mathrm{m}}\right)^{-\frac{1}{2}}\frac{\mathrm{dx_{cl}}}{\mathrm{dt}}. \tag{16}$$

With this, we encounter that the determinant of B must be zero and, thus, the amplitude in Eq. (10) seems to diverge. This is a direct consequence of the time invariance of the system. Stepping a little bit back, but now being aware that one of the eignevalues is zero, Eq. (11) can be written as (see [8]):

$$(\det(B))^{-1/2} = \int \frac{dc_0}{\sqrt{2\pi\hbar}} \int \prod_{n>0} \frac{dc_n}{\sqrt{2\pi\hbar}}\, e^{-\frac{1}{2\hbar}\sum_{n>0}\lambda_n c_n^2}, \tag{17}$$

where the $(2\pi\hbar)^{-1/2}$ are just normalization factors.

The second integration in Eq. (17) is a Gaussian and it can be calculated, giving as a result a determinant that does not take into account the zero eigenvalue. So we see more clearly now where the divergence does come from: the first integration is not a Gaussian and, thus, it's not damped. As said, this is a consequence of the time invariance and, for that reason, should be solvable be changing the integration variable from dc_0 to $d\tau_c$ (an integration over all the possible centers of the instanton). Recalling Eq. (9), if we vary c_n by Δc_0, we get the change in $x(\tau)$: $\Delta x(\tau) = \psi_0(\tau)\Delta c_0$. And, the change in $x(\tau)$ due to a change in the center of the instanton (namely, a change in τ_c) can also be obtained by $\Delta x(\tau) = \frac{dx}{d\tau_c}\Delta\tau_c$. Comparing both expressions, one can see that

$$\frac{dc_0}{d\tau_c} = \left(\frac{S_0}{m}\right)^{\frac{1}{2}}. \tag{18}$$

So the determinant in Eq. (17) is finally written as

$$(\det(B))^{-1/2} = \frac{\left(\frac{S_0}{m}\right)^{\frac{1}{2}}}{\sqrt{\det{}'\left(-m\frac{d^2}{d\tau^2} + V''(x_{cl})\right)}} \cdot \frac{1}{\sqrt{2\pi\hbar}} \int_{-\frac{T}{2}}^{\frac{T}{2}} d\tau_c, \tag{19}$$

where det' stands for the determinant of the operator without the zero eigenvalue (i.e. only the second integration in Eq. (17)) and is the last term left to calculate.

The complete calculus can be done by different methods, which are plenty described in [7], [8]. In most of them, it is done for a quartic potential, but the procedure is the same as for the cubic potential.

Finally, plugging all the calculations into Eq. (10), it is obtained the transition amplitude for one instanton:

$$\left\langle 0\middle|e^{-\frac{1}{\hbar}TH}\middle|0\right\rangle = \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{w\mathrm{T}}{2}}\, r\int_{-\mathrm{T}/2}^{\mathrm{T}/2} d\tau_c, \qquad (20)$$

with

$$r = 4i\sqrt{\frac{wm}{\pi\hbar}}\, w x_0 e^{-\frac{S_0}{\hbar}}. \qquad (21)$$

As said, Eq. (20) corresponds only to the contribution of one instanton (just one bounce). However, the physical observable would not change if n instantons contributed to the phenomenon (i.e. n bounces occurred). Then, if we want to compute the total transition amplitude, we must sum over all possible contributions, from one instanton to infinity. For instance, for an *n-instanton* contribution, each instanton will be centered at a different $\tau_c^{(i)}$ (all of them between the initial time and the final time): $-\frac{\mathrm{T}}{2} \leq \tau_c^{(n)} \leq \cdots \leq \tau_c^{(i)} \leq \cdots \leq \frac{\mathrm{T}}{2}$

Thus, the integral over $d\tau_c$ becomes for this n-instanton:

$$\int_{-\frac{\mathrm{T}}{2}}^{\frac{\mathrm{T}}{2}} d\tau_c^{(1)} \ldots \int_{-\frac{\mathrm{T}}{2}}^{\tau_c^{(n-1)}} d\tau_c^{(n)} = \frac{\mathrm{T}^n}{n!}. \qquad (22)$$

Considering that the r comes from the calculus of one instanton, for n instantons it will be simply r^n. The total amplitude will be then:

$$\left\langle x_i = 0\middle|e^{-\frac{1}{\hbar}TH}\middle|x_f = 0\right\rangle = \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{w\mathrm{T}}{2}} \sum_{n=1}^{\infty}\frac{(r T)^n}{n!}. \qquad (23)$$

And this sum can be done:

$$\left\langle x_i = 0\middle|e^{-\frac{1}{\hbar}TH}\middle|x_f = 0\right\rangle = \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{w\mathrm{T}}{2}} e^{rT}. \qquad (24)$$

Recalling from Eq. (21) that r is imaginary; we see that the total amplitude is imaginary too.

This should not surprise us, since from Eq. (16) we know that the eigenfunction with zero eigenvalue is proportional to the classical velocity of the particle. In *Fig. 4* is shown this function and it's obvious that it has a node. As it is widely known from quantum mechanics, the eigenfunction with the lowest eigenvalue has no nodes. So, if ψ_0 is the eigenfunction with zero eigenvalue, but there is a function with lower eigenvalue (thus negative), it's obvious that the determinant in Eq. (10) will be negative and, in consequence, the total amplitude will be imaginary.

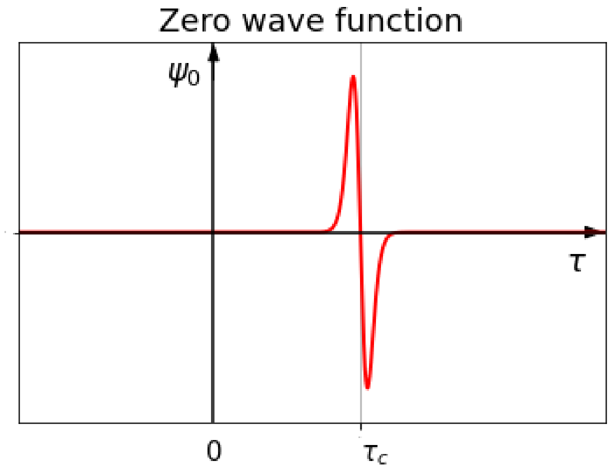

FIG.4: Eigenfunction of the zero eigenvalue over time. It has a node at τ_c which, remember, can take any value.

Now that we have the total amplitude, let us recover Eq. (7). If we suppose that the main contribution of it comes from the first term, we get:

$$\left\langle 0\middle|e^{-\frac{1}{\hbar}TH}\middle|0\right\rangle \simeq e^{-\frac{E_0 T}{\hbar}}\, |\langle n=0|x=0\rangle|^2. \qquad (25)$$

By comparing Eqs. (24) and (25), we can see that ([11]):

$$\mathrm{E}_0 = \frac{w\hbar}{2} - \hbar r. \qquad (26)$$

We see that the energy has an imaginary part. This is related to the decaying rate of the metastable state, as it follows.

Knowing that the evolution of the wave function (back to real time) is given by

$$|\psi_0(t)\rangle \propto e^{-\frac{iE_0 t}{\hbar}}|\psi_0(0)\rangle. \qquad (27)$$

And, substituting (26) into (27),

$$|\psi_0(t)\rangle \propto e^{-Im(r)\cdot t}\, e^{-\frac{iw}{2}t}|\psi_0(0)\rangle. \qquad (28)$$

As the first exponential has a real and positive argument, we can easily see that it is a damping exponential. So, $k \equiv Im(r)$ corresponds to what is called the decaying rate:

$$k = 4\sqrt{\frac{wm}{\pi\hbar}}\, w x_0 e^{-\frac{8mw(x_0)^2}{15\hbar}}. \qquad (29)$$

Result that can actually be obtained, by a slightly different method (used in [12] for the double well case). It can be studied the dependence with the different parameters (w,m,x_0). In *Fig. 5* is shown as an example how this rate increases at first with increasing w but then rapidly decreases, as the exponential damping gains importance. In *Fig. 6* a density plot is shown where both axis correspond to the parameters that may affect the decaying rate.

By taking the squared module of Eq. (24), [10], we can obtain the probability of the transition as a function of time.

$$P_{x_i\to x_f}(\mathrm{T}) = \left|\left\langle 0\middle|e^{-\frac{1}{\hbar}TH}\middle|0\right\rangle\right|^2 = \left(\frac{mw}{\pi\hbar}\right) e^{-w\mathrm{T}}. \qquad (30)$$

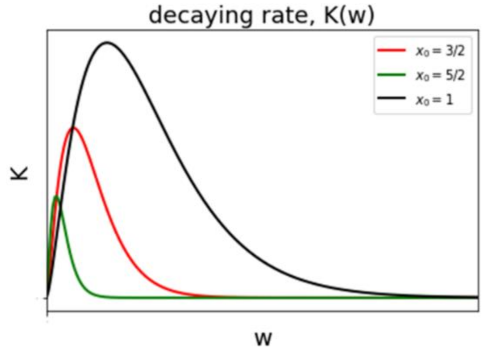

FIG.5: Evolution of the decaying rate as a function of the frequency w.

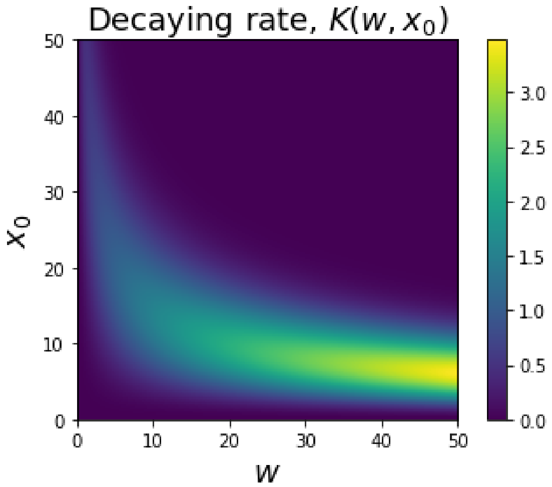

FIG.5: Density plot of the decaying rate in function of both parameters (w and x_0).

VI. Conclusions

To compute the Feynmann path integral associated to the transition amplitude, we used the saddle-point method, which demands to make an expansion around the local extreme of the action. However, as the action had no local minimum (firstly, there is no classical trajectory for such potential) we had to perform a Wick rotation (and thus, work in imaginary time) in order to be able to continue.

We found in sections IV and V that the classical trajectory takes place in sudden and short intervals of time (instantons) and that more than one of these can happen, as it is irrelevant to the final result if one or *n* of these instantons contribute.

The fact that the amplitude found is imaginary traduces directly to the damping of the state and, thus, to the metastability of the system. From this the decaying rate, K, of the state could be obtained. The lifetime of the system can be obtained by just computing the inverse of K. With the transition probability, one can see that it decreases with the transition time, fact that is completely logic, since the longer it is the transition time, the less likely is tunnelling.

VII. Acknowledgments

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